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SOLID STATE CHEMISTRY

CONTENTS

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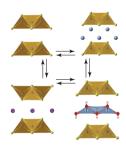
Editorial

Solid state chemistry of energy-related materials Susan E. Latturner and Michael Shatruk page 1

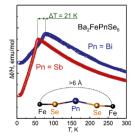
Regular Articles

The intercalation chemistry of layered iron chalcogenide superconductors

Hector K. Vivanco and Efrain E. Rodriguez *page 3*



Synthesis, crystal structure, and magnetic properties of quaternary iron selenides: Ba₂FePnSe₅ (Pn=Sb, Bi) Jian Wang, Joshua T. Greenfield and Kirill Kovnir page 22

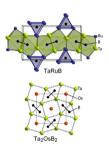


In Ba₂FeSbSe₅ and Ba₂FeBiSe₅ the magnetic interactions between Fe³⁺ centers, which are at least 6 Å apart from each other, are mediated by superexchange interactions.

Regular Articles—Continued

New ternary tantalum borides containing boron dumbbells: Experimental and theoretical studies of Ta₂OsB₂ and TaRuB

Mohammed Mbarki, Rachid St. Touzani, Christian W.G. Rehorn, Fabian C. Gladisch and Boniface P.T. Fokwa page 28

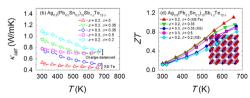


The two new ternary tantalum borides, Ta_2OsB_2 and TaRuB, have been discovered. Their crystal structures contain boron dumbbells, which are the strongest bonds. Peirls distortion is found responsible for Os_2 -dumbbells formation in Ta_2OsB_2 . Ta_2OsB_2 and TaRuB are Pauli paramagnet and potential superconductors.

Thermoelectric properties of p-type $Ag_{1-x}(Pb_{1-y}Sn_y)_mSb_{1-z}$ Te_{m+2}

Kyunghan Ahn, Huijun Kong, Ctirad Uher and Mercouri G. Kanatzidis

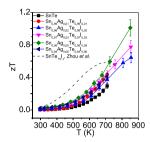
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The $Ag_{1-x}(Pb_{1-y}Sn_y)_mSb_{1-z}Te_{m+2}$ system defines a complex and flexible class of tunable thermoelectric class of materials with high performance.

AgI alloying in SnTe boosts the thermoelectric performance via simultaneous valence band convergence and carrier concentration optimization

Ananya Banik and Kanishka Biswas page 43

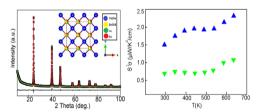


Significant decrease in hole concentration and reduction of the energy separation between light and heavy hole valence bands resulted in a maximum thermoelectric figure of merit, zT, of ~1.05 at 860 K in high quality crystalline ingot of p-type $Sn_{0.95}Ag_{0.05}Te_{0.95}I_{0.05}$.

Synthesis, crystal structure and electrical properties of the tetrahedral quaternary chalcogenides CuM₂InTe₄ (M=Zn, Cd)

George S. Nolas, M. Shafiq Hassan, Yongkwan Dong and Joshua Martin

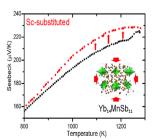
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The structural, optical and electrical properties of the quaternary chalcogenides $\text{CuZn}_2\text{InTe}_4$ and $\text{CuCd}_2\text{InTe}_4$ are reported for the first time. The unique crystal structure allows for relatively good electrical transports and therefore potential for thermoelectric applications.

Effects of Sc and Y substitution on the structure and thermoelectric properties of Yb₁₄MnSb₁₁

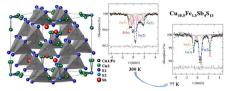
Jason H. Grebenkemper, Sebastian Klemenz, Barbara Albert, Sabah K. Bux and Susan M. Kauzlarich *page* 55



Chemical pressure of the Sc substituted $Yb_{14}MnSb_{11}$ provides a viable method for enhancing the Seebeck coefficient.

Role of iron in synthetic tetrahedrites revisited

Daria I. Nasonova, Igor A. Presniakov, Alexei V. Sobolev, Valeriy Yu. Verchenko, Alexander A. Tsirlin, Zheng Wei, Evgeny V. Dikarev and Andrei V. Shevelkov *page 62*

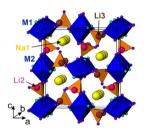


Synthetic iron-containing tetrahedrites, $Cu_{12-x}Fe_xSb_4S_{13}$, display a variable valence state and role of iron. At low iron content two nonequivalent and non-interacting Fe^{3+} cations occur. At higher levels of substitution, room-temperature Mössbauer spectra indicate the electron hopping between part of Fe^{3+} and Fe^{2+} centers, which freezes out upon cooling down to 77 K, whereas the rest of iron atoms exists as valence-localized Fe^{3+} and Fe^{2+} cations.

Synthesis, structure and electrochemical properties of LiNaCo_{0.5}Fe_{0.5}PO₄F fluoride-phosphate

Stanislav S. Fedotov, Sergey M. Kuzovchikov, Nellie R. Khasanova, Oleg A. Drozhzhin, Dmitriy S. Filimonov, Olesia M. Karakulina, Joke Hadermann, Artem M. Abakumov and Evgeny V. Antipov

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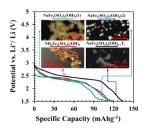


The ball-polyhedral representation of the LiNaCo $_{0.5}$ Fe $_{0.5}$ PO $_{4}$ F crystal structure. The MO $_{4}$ F $_{2}$ units are depicted as blue octahedra, PO $_{4}$ units as orange tetrahedra, sodium atoms are designated as yellow (Na1), lithium – red and brown (Li2, Li3 resp.), fluorine – green, oxygen – violet spheres.

Kagomé lattices as cathode: Effect of particle size and fluoride substitution on electrochemical lithium insertion in sodium- and ammonium Jarosites

Prashanth Sandineni, Hooman Yaghoobnejad Asl and Amitava Choudhury

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Discharge capacity of jarosite phases as a function of particle size and fluoride substitution.

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